

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 139 days

Global applicability domain: Outside

Local applicability domain index: 9.51e-02

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Octahydro-exo-4,7-methano-1H-indene</div> <div>Measured: 8090000</div> <div>Predicted: 636</div>	<div>Image not found</div> <div>9-Ethyl-9H-fluorene</div> <div>Measured: 2330</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>Dibenzothiophene</div> <div>Measured: 3830</div> <div>Predicted: 44.6</div>
<div>Image not found</div> <div>Indeno(1,2,3-cd)pyrene</div> <div>Measured: 630000</div> <div>Predicted: 325</div>	<div>Image not found</div> <div>11H-Benzo[a]fluorene</div> <div>Measured: 88900</div> <div>Predicted: 121</div>	